LETTER TO THE EDITOR

New field theory formulation of localised states in disordered systems

S M Girvin†, R W Rendell‡§ and G W Bryant†

- † Surface Science Division, National Bureau of Standards, Washington, DC 20234, USA
- ‡ Electron Physics Group, National Bureau of Standards, Washington, DC 20234, USA

Received 10 July 1981

Abstract.We present a new field theoretic formulation of the quantum mechanics of disordered systems. The problem is converted to an explicit field theory by changing variables in the functional integral over all random potentials to an integral over all possible wavefunctions. Unlike previous formulations this field theory has the novel feature of having the 'right' sign for the coefficient of the φ^4 term. Thus the important excitations are kinks rather than instantons. In addition, it exhibits singular solutions with finite action. The method is illustrated with an exact calculation of the asymptotic density of states in a one-dimensional gaussian white noise potential.

There has been a great interest in recent years in the quantum mechanics of random potentials. Typically one would like to calculate some property of the eigenvalues and eigenfunctions averaged over the ensemble of random potentials. For example, the average Green's function has spectral density

$$A_{xy}(E) = \frac{1}{Z} \int DV P(V) 2\pi \sum_{i} \Psi_{i}^{*}(x) \Psi_{i}(y) \delta(E - E_{i})$$

where P is the probability distribution for the potential V, Ψ_i is the *i*th eigenfunction with eigenvalue E_i and Z is the partition function. Considerable effort has recently gone into the question of how to apply the techniques of quantum field theory and statistical mechanics to this type of problem. In a typical phase transition problem one is interested in correlation functions for some field S of the form

$$G_{xy} = Z^{-1} \int DS P(S) S(x) S(y).$$

Unfortunately the random potential problem does not have this form since the functional integral is over the potential V, whereas the correlations of interest are between wavefunctions. The main thrust of efforts to circumvent this difficulty have taken advantage of the formal equivalence (Ma 1972, Thouless 1975) (term by term in perturbation theory) between the random (gaussian distributed) potential problem and the $n \to 0$ limit (replica trick) of an n-component Landau-Ginzburg field theory. Cardy (1978) and Brézin and Parisi (1980) have used this equivalence to calculate the ensemble averaged density of states in the weak coupling regime (deeply localised states). Wegner (1979a,

§ NRC/NBS Postdoctoral Fellow.

b, 1980) and others (Harris and Lubensky 1980, 1981, McKane and Stone 1981) have extensively developed the replica field theory formulation of calculations for the four-point correlation function which yields information about localisation and transport. There has been much interest in the fact that the coefficient of the φ^4 term in the Lagrangian density has the 'wrong' sign, so that the important excitations in this problem are non-perturbative instanton solutions of the classical Landau-Ginzburg equation.

The use of non-perturbative instanton solutions was justified (at least in the density of states calculation) by Houghton and Schäfer (HS) (1979) (see also Houghton et al 1980). They avoided the $n \to 0$ trick by formulating a direct variational principle for the problem. Variational formulations have been presented previously (Zittartz and Langer 1966, Langer 1967, Halperin and Lax 1966, 1967, Edwards 1970, Abram and Edwards 1972, Thouless 1975, Thouless and Elzain 1978); however, the HS method takes advantage of field theoretic techniques for dealing with nonlinear quantum systems. Because they were forced to invoke second-order perturbation theory in evaluating fluctuations about the extremal potential, HS did not obtain an explicit field theory. It is thus difficult to develop a systematic expansion in the coupling constant with their scheme. Schäfer and Wegner (1980) pointed out the importance of this difficulty and show that the perturbation theory is at least somewhat simpler in lattice models.

We present here preliminary results of a new approach to the problem which avoids the replica trick and the necessity of perturbation theory and reduces the problem to an explicit field theory which is amenable to analysis using standard techniques. One of the novel features of this field theory is that the coefficient of the φ^4 term has the 'right' sign. There are also several other extremely interesting features which we shall discuss. As a simple illustration of the procedure we calculate the asymptotically exact density of states in a one-dimensional gaussian white noise potential. More extensive results will be reported elsewhere (Rendell et al 1981).

Consider the density of states in one dimension for asymptotically deep energies, $\omega \to -\infty$. The ensemble average is

$$\rho(\omega) = L^{-1}Z^{-1} \int DV \exp(-\tilde{S}[V]) \sum_{i} \delta(\omega - E_{i})$$
 (1)

where L is the sample length, E_i is the *i*th eigenvalue of the random potential V, \hat{S} is the action

$$\tilde{S} = \frac{1}{2\sigma^2} \int_{-L/2}^{L/2} dx V^2(x)$$
 (2)

and Z is the partition function. The mean square potential σ^2 is a measure of the disorder. The main difficulty in evaluating equation (1) is the delta function which requires solving the Schrödinger equation with a random potential in order to determine the eigenvalues. The key to our approach is the observation that given a wavefunction Ψ and an eigenvalue ω it is trivial to invert the Schrödinger equation to find the corresponding potential $(\hbar^2/2m=1)$:

$$V(x) = \omega + \Psi''/\Psi. \tag{3}$$

It is therefore desirable to change variables in equation (1) so that the integration is over all possible eigenfunctions and eigenvalues rather than all potentials. The functional integral will then have the form of a statistical mechanics problem. Because of the invariance of equation (3) with respect to the scale of Ψ , it is convenient to make use of the dimensionless field g defined by

$$g(x) = \frac{1}{\alpha} \frac{\Psi'}{\Psi} \tag{4}$$

where $\alpha = (-\omega)^{1/2}$. We also scale to a dimensionless length coordinate $x \to \alpha x$ so that equation (3) becomes

$$V(x) = -\omega(-1 - g' + g^2). \tag{5}$$

The corresponding action may be split into the sum of two terms

$$\tilde{S} = K(S + S_{B}) \tag{6}$$

where $K = |\omega|^{3/2}/2\sigma^2$, S is the action for an ordinary φ^4 theory (with positive self-coupling)

$$S = \int_{-l/2}^{l/2} dx [(g')^2 - 2g^2 + g^4 + 1]$$
 (7)

 $l=\alpha L$, and $S_{\rm B}$ is a perfect derivative term. It is assumed that the potential vanishes outside the interval [-l/2, l/2] so that the eigenfunction boundary condition is $g(\pm l/2)=\pm 1$. Thus the field is restricted to topological charge +1 and the perfect derivative term integrates to $S_{\rm B}=\frac{8}{3}$.

Equation (1) may now be written

$$\rho(\omega) = L^{-1}Z^{-1} \int d\Omega \int' Dg J(\Omega, g) \exp\{-K(\Omega)(S[g] + \frac{8}{3})\} \delta(\omega - \Omega)$$
 (8)

where J is the Jacobian for the change of variables from the field V to the field g plus the eigenvalue variable Ω . The constraint that g corresponds to an eigenfunction satisfying appropriate boundary conditions removes one degree of freedom which is compensated by the extra integration over Ω . This constraint is indicated by a prime on the integral. The complicated delta function is now trivial and one obtains

$$\rho(\omega) = \exp(-8K/3) L^{-1}Z^{-1} \int_{0}^{T} Dg J(\omega; g) \exp(-KS[g]).$$
 (9)

A similar change of variables may be made in the partition function

$$Z = \int Dg \ H(\omega; g) \ \exp(-KS[g]). \tag{10}$$

Because there is no delta function as in equation (1) to simplify the eigenvalue integration, we have chosen to remove the constraint on g and hence have eliminated the eigenvalue integration degree of freedom. Thus the Jacobian in equation (10) differs from that in equation (9).

The required Jacobians may be exactly evaluated (Rendell et al 1981) by treating the real line as a discrete lattice and explicitly evaluating the determinant of the Jacobian matrix by a direct expansion in minors. In the continuum limit one obtains

$$J = \frac{Q}{|\omega|\alpha} \left\{ \cosh \left[\int_{-l/2}^{l/2} dx \ g(x) \right] + \int_{-l/2}^{l/2} dy \ \exp \left[- \int_{-l/2}^{l/2} dy \ \operatorname{sgn}(y - x) \ g(x) \right] \right\}$$
(11)

where Q is a (formally infinite) constant. This may be very simply expressed in terms of the wavefunction as

$$J = \frac{Q}{|\omega|} \frac{1}{|\Psi(-l/2)|\Psi(l/2)|}.$$
 (12)

Likewise we have

$$H = Q \exp \left[- \int_{-l/2}^{l/2} dx \ g(x) \right]. \tag{13}$$

Equations (9)–(13) constitute a reduction of the problem to an *explicit* field theory. It is clear however that the Jacobian J introduces complicated long-range interactions into the problem.

Having established the field theory we begin our analysis by seeking the classical extremal solutions. In the asymptotic regime $(K \to \infty)$ one may neglect the variation of the Jacobian relative to the variation of S. Treating J and H as constants leaves one with ordinary φ^4 theory and so the extremal field satisfies the usual Landau-Ginzburg equation

$$-1/2g'' - g + g^3 = 0. (14)$$

Using equation (4), equation (14) can be shown to be completely equivalent to the instanton equation obtained by HS. Thus our neglect of the variation of the Jacobian is equivalent to the neglect by HS of the variation of the measure of the delta function in equation (1).

The simplest solution to (14) which has the required topological charge is the one kink solution, $g_0(x) = \tanh(x)$. This has action $S = \frac{8}{3}$ and corresponds to the wavefunction $\Psi(x) = [\sqrt{2} \cosh(x)]^{-1}$. The partition function will be evaluated in the vicinity of the extremal field g(x) = -1 for which $S = S_B = 0$. Evaluation of the Jacobians at the extremal fields using equations (12) and (13) yields $J/H = 1/2 |\omega|$.

We are now in a position to evaluate the functional integral in equation (9) in terms of the fluctuations about the classical solution using standard field theoretic techniques (Goldstone and Jackiw 1975, Rajaraman 1975, Coleman 1977). Integration over the collective coordinate describing the kink position yields a factor $(4/3)^{1/2}\alpha L$. The 'free energy' for the kink is found to be

$$F = \frac{8}{3}K + \frac{1}{2}\ln(2\pi/6K) + (\ln(24K/2\pi))$$
 (15)

where the first term is the classical energy, the second is due to the kink breather mode, and the third is the change in the 'phonon' free energy due to the presence of the kink. Because the kink automatically satisfies the boundary conditions placed on g, equation (15) was derived requiring the fluctuations to vanish at the boundaries. There is no such constraint on the field in the partition function so that there is one more integration over the zero wavevector phonon mode (which does not vanish at the boundaries). This gives an extra factor of $(2\pi/8K)^{1/2}$ in the denominator. Combining all these factors together, equation (9) becomes

$$\rho(\omega) = \frac{8\alpha K}{\pi |\omega|} \exp(-16K/3) = \frac{4|\omega|}{\pi \sigma^2} \exp(-16K/3)$$
 (16)

which agrees exactly with the known asymptotic result (Frisch and Lloyd 1960, Halperin 1965, Zittartz and Langer 1966).

The above result is based on the assumption that only a single kink is present and hence is valid only for infinitesimal disorder. For finite disorder one must consider a gas of kinks and antikinks. We are currently investigating this question and briefly outline here only the main features involved. A fuller discussion of the statistical mechanics of this system will be presented elsewhere (Rendell *et al* 1981).

In seeking corrections to the asymptotic result, it is necessary to consider the Jacobian

J in greater detail since it produces non-local interactions in the field theory. We begin by considering the simplest multikink case which consists of two kinks separated by an antikink. We again ignore the variation of the Jacobian when calculating the *shape* of the kinks and consider its effect only on the *interaction* of the kinks. This leads to a long-range attractive potential $v_{xy} \sim -|x-y|$ between the kinks which confines them. For a general cluster of n kinks and n-1 antikinks one finds that the potential energy depends primarily on the separation of the end kinks.

Notice that up to now we have implicitly assumed that the wave function Ψ has no nodes. It is clear from equation (4) that if Ψ has a node the field g will have a singularity. We have found a new solution to the Landau–Ginzburg equation (14) which corresponds to the presence of a node in Ψ

$$g(x) = -\coth(x). \tag{17}$$

We refer to this as a chirp because of its singular nature. Such a singular solution would normally have infinite action but in this case the action vanishes because of the perfect derivative terms in the Lagrangian which were mentioned earlier. Because g is not integrable in the presence of a chirp it is impossible to turn the perfect derivatives into a simple boundary term as in equation (6).

When evaluating fluctuations about the ordinary kink, it is well known that the kink presents a reflectionless potential to the 'phonons'. One of the interesting features of the chirp is that it presents an infinite barrier and is therefore transmissionless. This means that a pair of chirps traps of gas of phonons between them. The pressure of this gas will contribute to a long-range interaction between the chirps.

In summary we have presented a new approach to the quantum mechanics of random potentials. The key feature is that instead of ensemble averaging over all possible random potentials we change variables to the ensemble of all possible random wavefunctions. We have presented preliminary results for the calculations of a simple quantity—the asymptotic density of states in one dimension. We find that this variable change allows the problem to be reduced to an explicit field theory with a repulsive φ^4 self-interaction plus non-local interactions. The physical sector is constrained to topological charge +1. This field theory exhibits several novel features including the existence of singular classical solutions with finite action. It is hoped that the present formulation will allow the systematic calculation of corrections to the asymptotic results and can be extended to the study of higher correlation functions.

We are extremely grateful to W Caswell, M Ogilve, J Schonfeld and M Danos for valuable assistance in our efforts to come to grips with field theoretic techniques.

References

Abram R A and Edwards S F 1972 J. Phys. C: Solid State Phys. 5 1183 Brézin E and Parisi G 1980 J. Phys. C: Solid State Phys. 13 L307

Cardy J L 1978 J. Phys. C: Solid State Phys. 11 L321

Coleman S 1977 Proc. 14th Int. School of Subnuclear Physics, Ettore Majorana, Erice 1975 ed A Zichichi (New York: Plenum)

Edwards S F 1970 J. Non-Cryst. Solids 4 417 Frisch H L and Lloyd S P 1960 Phys. Rev. 120 1175 Goldstone J and Jackiw R 1975 Phys. Rev. D11 1486 Halperin B I 1965 Phys. Rev. 139 104

Letter to the Editor L886

Halperin B I and Lax M 1966 Phys. Rev. 148 722

--- 1967 Phys. Rev. 153 802

Harris A B and Lubensky T C 1980 Solid State Commun. 34 343

- 1981 Phys. Rev. B23 2640

Houghton A and Schäfer L 1979 J. Phys. A: Math Gen. 12 1309

Houghton A, Schäfer L and Wegner F J 1980 Phys. Rev. B 22 3598

Langer J S 1967 Ann. Phys. 41 108

Ma S K 1972 unpublished

McKane A J and Stone M 1981 Ann. Phys. 131 36

Rajaraman R 1975 Phys. Rep. 21 227

Rendell R W, Girvin S M and Bryant G W 1981 to be published

Schäfer L and Wegner F 1980 Z. Phys. B39 281

Thouless D J 1975 J. Phys. C: Solid State Phys. 8 1803

Thouless D J and Elzain M E 1978 J. Phys. C: Solid State Phys. 11 3425

Wegner F 1979a Z. Phys. B35 207

—— 1979b Phys. Rev. B19 783 —— 1980 Z. Phys. B 36 209

Zittartz J and Langer J S 1966 Phys. Rev. 148 741